

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester  
145348-23-8 | DTXSID20162992

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 4.57e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.44e-01

Confidence level: 3.14e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,5-Dichlorodiphenyl ether</div> <div>Measured: 2.78e-06</div> <div>Predicted: 9.53e-04</div>	<div>Image not found</div> <div>Kinoprene</div> <div>Measured: 1.50e-08</div> <div>Predicted: 1.35e-05</div>	<div>Image not found</div> <div>Dibenzofuran, 2,3,6,7-tetrachloro-</div> <div>Measured: 5.25e-07</div> <div>Predicted: 2.06e-08</div>
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